Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 10:58 pm BST

PDB ID	:	1DFO
Title	:	CRYSTAL STRUCTURE AT 2.4 ANGSTROM RESOLUTION OF E. COLI SERINE HYDROXYMETHYLTRANSFERASE IN COMPLEX WITH GLYCINE AND 5-FORMYL TETRAHYDROFOLATE
Authors	:	Scarsdale, J.N.; Radaev, S.; Kazanina, G.; Schirch, V.; Wright, H.T.
Deposited on	:	1999-11-20
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

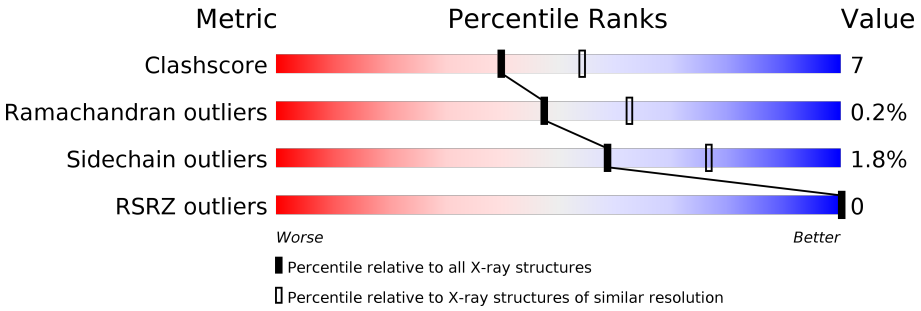
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	417	84% 14%
1	B	417	84% 15%
1	C	417	83% 16%
1	D	417	84% 14%

2 Entry composition

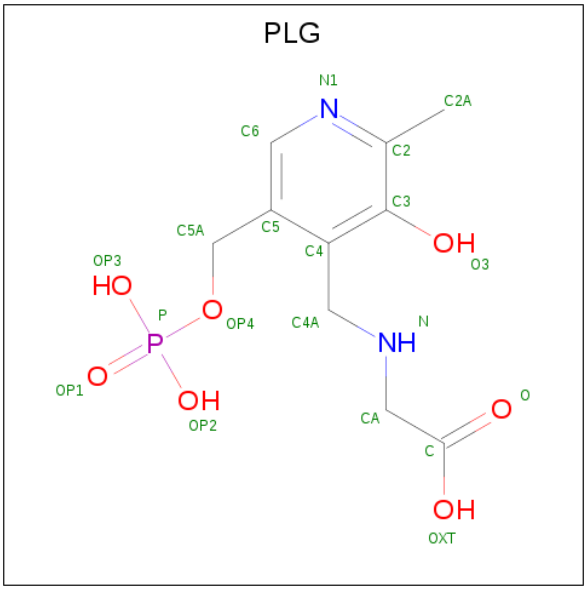
There are 4 unique types of molecules in this entry. The entry contains 13204 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3148	1995	541	598	14			
1	B	417	Total	C	N	O	S	0	0	0
			3167	2006	544	602	15			
1	C	417	Total	C	N	O	S	0	0	0
			3140	1989	539	597	15			
1	D	416	Total	C	N	O	S	0	0	0
			3145	1993	539	599	14			

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: $C_{10}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

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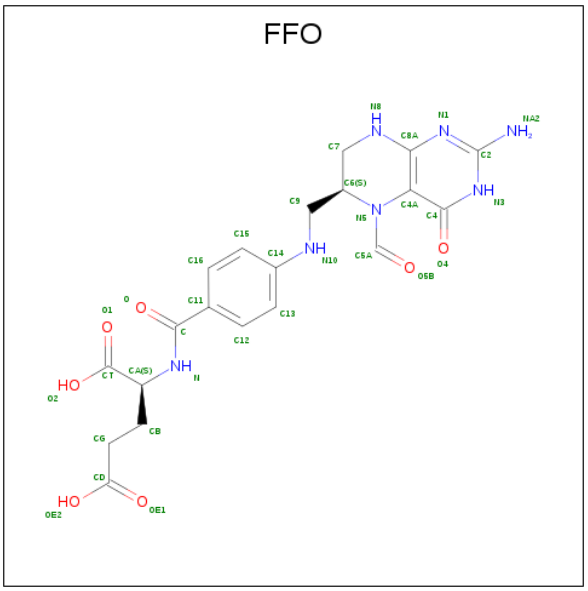
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 20 10 2 7 1	0	0
2	D	1	Total C N O P 20 10 2 7 1	0	0

- Molecule 3 is N-[4-({[(6S)-2-amino-5-formyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl }amino)benzoyl]-L-glutamic acid (three-letter code: FFO) (formula: $C_{20}H_{23}N_7O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 34 20 7 7	0	0
3	B	1	Total C N O 34 20 7 7	0	0
3	C	1	Total C N O 34 20 7 7	0	0
3	D	1	Total C N O 34 20 7 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	94	Total O 94 94	0	0
4	C	85	Total O 85 85	0	0

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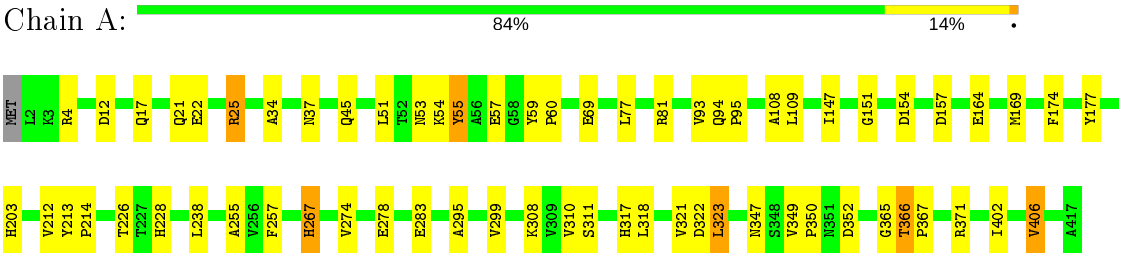
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	116	Total	O	0	0
			116	116		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

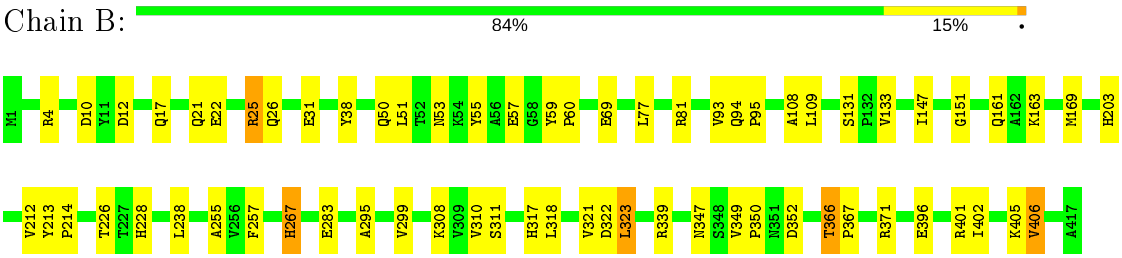
- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain A:



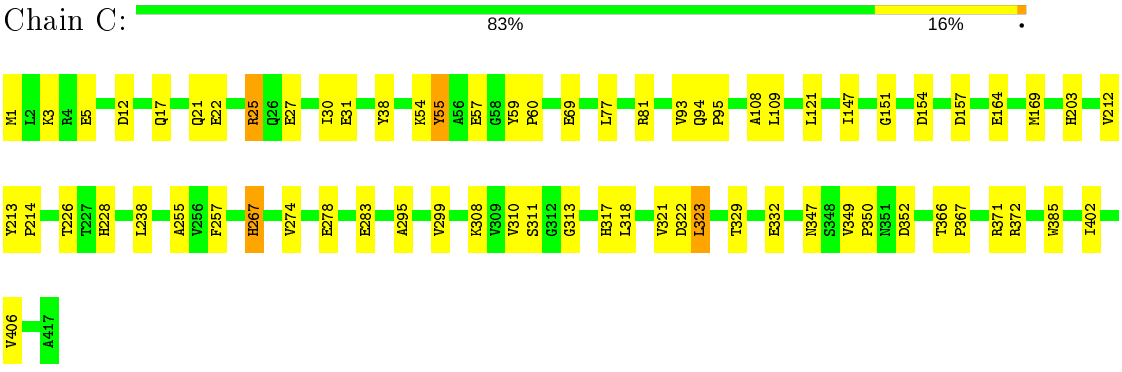
- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain B:



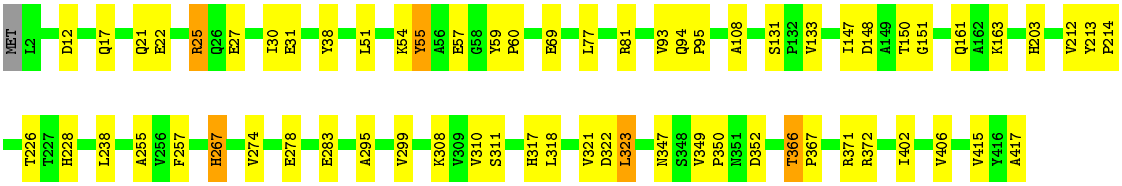
- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain C:



- Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain D:


MET L2 D12 Q17 Q21 E22 R25 Q26 E27 I30 E31 Y38 L51 K54 Y55 A56 E57 G58 Y59 P60 E69 L77 R81 V93 Q94 P95 A108 S131 P132 V133 I147 D148 A149 T150 G151 Q161 A162 K163 H203 V212 Y213 P214
T226 T227 H228 L238 A255 V256 F257 H267 V274 E278 E283 A295 V299 K308 V309 V310 S311 H317 L318 V321 D322 L323 N347 S348 V349 P350 N351 D352 T366 P367 R371 R372 I402 V406 V415 Y416 A417

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.46Å 172.24Å 95.05Å 90.00° 104.12° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 92.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.0 (20.00-2.40) 99.8 (92.18-2.40)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.174 , 0.196 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13204	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FFO, PLG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/3216	0.59	0/4363
1	B	0.32	0/3235	0.58	0/4386
1	C	0.32	0/3208	0.58	0/4356
1	D	0.33	0/3213	0.59	0/4360
All	All	0.32	0/12872	0.59	0/17465

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3148	0	3081	46	0
1	B	3167	0	3108	48	0
1	C	3140	0	3056	55	0
1	D	3145	0	3070	47	0
2	A	20	0	11	1	0
2	B	20	0	11	1	0
2	C	20	0	11	0	0
2	D	20	0	11	0	0
3	A	34	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	21	0	0
3	C	34	0	21	0	0
3	D	34	0	21	0	0
4	A	93	0	0	2	0
4	B	94	0	0	6	0
4	C	85	0	0	4	0
4	D	116	0	0	4	0
All	All	13204	0	12443	185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:HD3	1:C:164:GLU:OE2	1.77	0.84
1:C:77:LEU:O	1:C:81:ARG:HG3	1.80	0.82
1:D:77:LEU:O	1:D:81:ARG:HG3	1.80	0.81
1:B:77:LEU:O	1:B:81:ARG:HG3	1.82	0.80
1:A:164:GLU:OE2	1:D:163:LYS:HD3	1.81	0.79
1:A:77:LEU:O	1:A:81:ARG:HG3	1.84	0.77
1:B:339:ARG:HD2	4:B:753:HOH:O	1.91	0.71
1:A:267:HIS:CD2	1:A:267:HIS:H	2.11	0.69
1:D:267:HIS:CD2	1:D:267:HIS:H	2.12	0.66
1:B:267:HIS:H	1:B:267:HIS:CD2	2.11	0.66
1:C:267:HIS:CD2	1:C:267:HIS:H	2.12	0.65
1:A:17:GLN:O	1:A:21:GLN:HG3	1.99	0.63
1:C:17:GLN:O	1:C:21:GLN:HG3	1.99	0.63
1:B:17:GLN:O	1:B:21:GLN:HG3	2.00	0.61
1:D:366:THR:N	1:D:367:PRO:HD3	2.17	0.59
1:A:366:THR:N	1:A:367:PRO:HD3	2.18	0.58
1:B:366:THR:N	1:B:367:PRO:HD3	2.18	0.57
1:C:366:THR:N	1:C:367:PRO:HD3	2.19	0.57
1:B:161:GLN:HG2	4:B:698:HOH:O	2.06	0.56
1:A:366:THR:N	1:A:367:PRO:CD	2.68	0.56
1:A:12:ASP:OD2	1:B:81:ARG:NH2	2.38	0.56
1:B:366:THR:N	1:B:367:PRO:CD	2.69	0.56
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.72	0.55
1:C:366:THR:N	1:C:367:PRO:CD	2.70	0.55
1:A:45:GLN:HB2	4:A:767:HOH:O	2.06	0.55
1:D:366:THR:N	1:D:367:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:O	1:B:406:VAL:HG13	2.07	0.55
1:D:203:HIS:HD2	1:D:317:HIS:NE2	2.05	0.54
1:A:81:ARG:NH2	1:B:12:ASP:OD2	2.40	0.53
1:C:81:ARG:NH2	1:D:12:ASP:OD2	2.39	0.53
1:B:203:HIS:HD2	1:B:317:HIS:NE2	2.07	0.53
1:C:203:HIS:HD2	1:C:317:HIS:NE2	2.06	0.53
1:D:17:GLN:O	1:D:21:GLN:HG3	2.08	0.53
1:A:203:HIS:HD2	1:A:317:HIS:NE2	2.07	0.52
1:A:93:VAL:HG12	1:A:238:LEU:HD11	1.91	0.52
1:B:81:ARG:HD3	4:B:842:HOH:O	2.10	0.52
1:C:30:ILE:HG12	1:C:406:VAL:HG13	1.92	0.52
1:C:93:VAL:HG12	1:C:238:LEU:HD11	1.91	0.52
1:D:93:VAL:HG12	1:D:238:LEU:CD1	2.39	0.52
1:C:93:VAL:HG12	1:C:238:LEU:CD1	2.40	0.52
1:D:93:VAL:HG12	1:D:238:LEU:HD11	1.91	0.51
1:D:30:ILE:HG12	1:D:406:VAL:HG13	1.92	0.51
1:C:267:HIS:HD2	1:C:267:HIS:H	1.57	0.51
1:C:5:GLU:HG2	4:C:977:HOH:O	2.10	0.51
1:A:147:ILE:HD11	1:A:350:PRO:HG2	1.93	0.51
1:C:22:GLU:OE2	1:C:25:ARG:NH1	2.44	0.51
1:C:31:GLU:HG3	4:C:741:HOH:O	2.11	0.50
1:D:81:ARG:HD3	4:D:908:HOH:O	2.10	0.50
1:A:22:GLU:OE2	1:A:25:ARG:NH1	2.44	0.50
1:C:12:ASP:OD2	1:D:81:ARG:NH2	2.40	0.50
1:C:318:LEU:C	1:C:318:LEU:HD12	2.32	0.50
1:A:93:VAL:HG12	1:A:238:LEU:CD1	2.41	0.50
1:A:267:HIS:HD2	1:A:267:HIS:H	1.57	0.50
1:B:267:HIS:H	1:B:267:HIS:HD2	1.57	0.50
1:C:147:ILE:HD11	1:C:350:PRO:HG2	1.93	0.49
1:C:385:TRP:HB3	1:C:402:ILE:HD12	1.93	0.49
1:B:93:VAL:HG12	1:B:238:LEU:HD11	1.93	0.49
1:A:53:ASN:HA	4:A:643:HOH:O	2.13	0.49
1:C:1:MET:HE3	1:C:3:LYS:HD3	1.94	0.49
1:B:93:VAL:HG12	1:B:238:LEU:CD1	2.42	0.48
1:D:147:ILE:HD11	1:D:350:PRO:HG2	1.96	0.48
1:B:57:GLU:HB3	1:B:257:PHE:CZ	2.49	0.48
1:B:318:LEU:HD12	1:B:318:LEU:C	2.33	0.48
1:B:53:ASN:HA	4:B:660:HOH:O	2.13	0.48
1:B:147:ILE:HD11	1:B:350:PRO:HG2	1.95	0.48
1:C:317:HIS:HD1	1:C:317:HIS:H	1.61	0.48
1:D:267:HIS:H	1:D:267:HIS:HD2	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:O	1:D:415:VAL:O	2.32	0.48
1:D:318:LEU:C	1:D:318:LEU:HD12	2.34	0.48
1:C:81:ARG:HD3	4:C:864:HOH:O	2.13	0.47
1:B:317:HIS:HD1	1:B:317:HIS:H	1.62	0.47
1:D:57:GLU:HB3	1:D:257:PHE:CZ	2.49	0.47
1:A:321:VAL:HG12	1:A:323:LEU:CD1	2.45	0.47
1:B:349:VAL:O	1:B:352:ASP:HB2	2.14	0.47
1:C:212:VAL:HG12	1:C:212:VAL:O	2.14	0.47
1:D:402:ILE:O	1:D:406:VAL:HG23	2.14	0.47
1:A:318:LEU:C	1:A:318:LEU:HD12	2.34	0.47
1:C:213:TYR:CD1	1:C:214:PRO:HD2	2.50	0.47
1:A:317:HIS:H	1:A:317:HIS:HD1	1.62	0.47
1:C:147:ILE:HD12	1:C:151:GLY:HA2	1.97	0.47
1:D:22:GLU:OE2	1:D:25:ARG:NH1	2.48	0.46
1:D:212:VAL:HG12	1:D:212:VAL:O	2.15	0.46
1:A:57:GLU:HB3	1:A:257:PHE:CZ	2.50	0.46
1:C:121:LEU:HD13	4:C:656:HOH:O	2.14	0.46
1:D:317:HIS:HD1	1:D:317:HIS:H	1.62	0.46
1:A:213:TYR:CD1	1:A:214:PRO:HD2	2.50	0.46
1:D:349:VAL:O	1:D:352:ASP:HB2	2.16	0.46
1:B:108:ALA:HB2	1:B:255:ALA:HB2	1.97	0.46
1:B:226:THR:HB	1:B:228:HIS:CE1	2.50	0.46
1:D:31:GLU:HG3	4:D:793:HOH:O	2.14	0.46
1:A:69:GLU:CD	1:A:69:GLU:H	2.19	0.46
1:B:212:VAL:O	1:B:212:VAL:HG12	2.15	0.46
1:C:402:ILE:O	1:C:406:VAL:HG23	2.16	0.46
1:D:226:THR:HB	1:D:228:HIS:CE1	2.51	0.46
1:B:213:TYR:CD1	1:B:214:PRO:HD2	2.51	0.45
1:A:22:GLU:HG2	1:B:51:LEU:CD2	2.45	0.45
1:A:402:ILE:O	1:A:406:VAL:HG13	2.16	0.45
1:B:22:GLU:OE2	1:B:25:ARG:NH1	2.49	0.45
1:B:321:VAL:HG12	1:B:323:LEU:CD1	2.47	0.45
1:C:108:ALA:HB2	1:C:255:ALA:HB2	1.98	0.45
1:B:4:ARG:NH1	1:B:50:GLN:OE1	2.46	0.45
1:D:310:VAL:O	1:D:311:SER:HB2	2.16	0.45
1:A:108:ALA:HB2	1:A:255:ALA:HB2	1.98	0.45
1:A:226:THR:HB	1:A:228:HIS:CE1	2.52	0.45
1:A:349:VAL:O	1:A:352:ASP:HB2	2.17	0.45
1:B:10:ASP:C	1:B:10:ASP:OD1	2.55	0.45
1:B:310:VAL:O	1:B:311:SER:HB2	2.17	0.45
1:B:267:HIS:N	1:B:267:HIS:CD2	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLU:H	1:B:69:GLU:CD	2.20	0.45
1:A:147:ILE:HD12	1:A:151:GLY:HA2	1.99	0.44
1:D:295:ALA:O	1:D:299:VAL:HG23	2.16	0.44
1:D:108:ALA:HB2	1:D:255:ALA:HB2	1.99	0.44
1:D:147:ILE:HD12	1:D:151:GLY:HA2	1.98	0.44
1:A:310:VAL:O	1:A:311:SER:HB2	2.18	0.44
1:D:27:GLU:O	1:D:372:ARG:NH2	2.39	0.44
1:D:308:LYS:HD3	1:D:322:ASP:HB3	1.99	0.44
1:A:109:LEU:HD12	1:A:169:MET:CE	2.48	0.44
1:C:226:THR:HB	1:C:228:HIS:CE1	2.53	0.44
1:B:295:ALA:O	1:B:299:VAL:HG23	2.18	0.44
1:D:213:TYR:CD1	1:D:214:PRO:HD2	2.52	0.44
1:D:94:GLN:N	1:D:95:PRO:CD	2.81	0.44
1:C:308:LYS:HD3	1:C:322:ASP:HB3	2.00	0.43
1:C:321:VAL:HG12	1:C:323:LEU:CD1	2.48	0.43
1:B:94:GLN:N	1:B:95:PRO:CD	2.81	0.43
1:D:274:VAL:O	1:D:278:GLU:HG3	2.18	0.43
1:C:69:GLU:CD	1:C:69:GLU:H	2.21	0.43
1:A:308:LYS:HD3	1:A:322:ASP:HB3	2.01	0.43
1:A:54:LYS:HD3	1:A:55:TYR:N	2.34	0.43
1:B:109:LEU:HD12	1:B:169:MET:CE	2.49	0.43
1:B:308:LYS:HD3	1:B:322:ASP:HB3	2.01	0.43
1:B:38:TYR:O	1:B:371:ARG:HD3	2.19	0.43
1:C:57:GLU:HB3	1:C:257:PHE:CZ	2.53	0.43
1:C:349:VAL:O	1:C:352:ASP:HB2	2.18	0.43
1:C:54:LYS:HD3	1:C:55:TYR:N	2.34	0.43
1:D:69:GLU:CD	1:D:69:GLU:H	2.22	0.43
1:B:31:GLU:HG3	4:B:686:HOH:O	2.19	0.43
1:C:274:VAL:O	1:C:278:GLU:HG3	2.19	0.43
1:D:161:GLN:HG2	4:D:831:HOH:O	2.19	0.43
1:C:1:MET:HE1	1:C:3:LYS:HE2	2.00	0.43
1:C:94:GLN:N	1:C:95:PRO:CD	2.82	0.43
1:C:30:ILE:CG1	1:C:406:VAL:HG13	2.49	0.42
1:B:147:ILE:HD12	1:B:151:GLY:HA2	2.00	0.42
1:C:22:GLU:HG2	1:D:51:LEU:CD2	2.48	0.42
1:C:283:GLU:H	1:C:283:GLU:CD	2.23	0.42
1:A:274:VAL:O	1:A:278:GLU:HG3	2.19	0.42
1:A:212:VAL:O	1:A:212:VAL:HG12	2.18	0.42
1:D:267:HIS:CD2	1:D:267:HIS:N	2.83	0.42
1:C:27:GLU:O	1:C:372:ARG:NH2	2.38	0.42
1:A:366:THR:H	1:A:367:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLN:N	1:A:95:PRO:CD	2.83	0.42
1:C:154:ASP:OD2	1:C:157:ASP:HB2	2.20	0.42
1:C:310:VAL:O	1:C:311:SER:HB2	2.20	0.42
1:D:321:VAL:HG12	1:D:323:LEU:CD1	2.50	0.42
1:D:38:TYR:O	1:D:371:ARG:HD3	2.19	0.42
1:C:1:MET:CE	1:C:3:LYS:HE2	2.50	0.42
1:C:267:HIS:N	1:C:267:HIS:CD2	2.83	0.42
1:A:37:ASN:OD1	1:A:371:ARG:HD2	2.21	0.41
1:A:59:TYR:HB3	1:A:60:PRO:HD2	2.02	0.41
1:B:59:TYR:HB3	1:B:60:PRO:HD2	2.03	0.41
1:A:51:LEU:CD2	1:B:22:GLU:HG2	2.51	0.41
1:C:59:TYR:HB3	1:C:60:PRO:HD2	2.02	0.41
1:D:31:GLU:HG2	4:D:561:HOH:O	2.20	0.41
1:D:59:TYR:HB3	1:D:60:PRO:HD2	2.01	0.41
1:A:174:PHE:CG	1:A:177:TYR:HB3	2.56	0.41
1:A:283:GLU:H	1:A:283:GLU:CD	2.24	0.41
1:D:148:ASP:HB3	1:D:150:THR:H	1.86	0.41
1:D:54:LYS:HD3	1:D:55:TYR:N	2.36	0.41
1:C:1:MET:SD	1:D:417:ALA:HB3	2.61	0.41
1:A:295:ALA:O	1:A:299:VAL:HG23	2.21	0.41
1:C:38:TYR:O	1:C:371:ARG:HD3	2.20	0.41
1:B:203:HIS:HE1	2:B:2001:PLG:O	2.04	0.41
1:B:401:ARG:O	1:B:405:LYS:HG3	2.21	0.41
1:C:295:ALA:O	1:C:299:VAL:HG23	2.20	0.41
1:D:283:GLU:H	1:D:283:GLU:CD	2.24	0.41
1:A:34:ALA:HA	1:A:365:GLY:HA3	2.03	0.40
1:C:299:VAL:HG11	1:C:313:GLY:HA2	2.03	0.40
1:D:131:SER:OG	1:D:133:VAL:HG22	2.21	0.40
1:C:109:LEU:HD12	1:C:169:MET:CE	2.50	0.40
1:A:154:ASP:OD2	1:A:157:ASP:HB2	2.22	0.40
1:A:203:HIS:HE1	2:A:1001:PLG:O	2.04	0.40
1:B:131:SER:OG	1:B:133:VAL:HG22	2.22	0.40
1:B:26:GLN:HG2	4:B:686:HOH:O	2.20	0.40
1:B:283:GLU:H	1:B:283:GLU:CD	2.24	0.40
1:C:329:THR:OG1	1:C:332:GLU:HG3	2.21	0.40
1:C:366:THR:H	1:C:367:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/417 (99%)	402 (97%)	11 (3%)	1 (0%)	47	62
1	B	415/417 (100%)	403 (97%)	11 (3%)	1 (0%)	47	62
1	C	415/417 (100%)	401 (97%)	14 (3%)	0	100	100
1	D	414/417 (99%)	401 (97%)	12 (3%)	1 (0%)	47	62
All	All	1658/1668 (99%)	1607 (97%)	48 (3%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	366	THR
1	A	366	THR
1	D	366	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/329 (97%)	314 (98%)	6 (2%)	57	75
1	B	323/329 (98%)	316 (98%)	7 (2%)	52	71
1	C	317/329 (96%)	312 (98%)	5 (2%)	62	79
1	D	319/329 (97%)	314 (98%)	5 (2%)	62	79
All	All	1279/1316 (97%)	1256 (98%)	23 (2%)	59	76

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	55	TYR
1	A	267	HIS
1	A	323	LEU
1	A	347	ASN
1	A	406	VAL
1	B	25	ARG
1	B	55	TYR
1	B	267	HIS
1	B	323	LEU
1	B	347	ASN
1	B	396	GLU
1	B	406	VAL
1	C	25	ARG
1	C	55	TYR
1	C	267	HIS
1	C	323	LEU
1	C	347	ASN
1	D	25	ARG
1	D	55	TYR
1	D	267	HIS
1	D	323	LEU
1	D	347	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
1	A	267	HIS
1	A	289	GLN
1	A	290	GLN
1	A	394	ASN
1	B	203	HIS
1	B	267	HIS
1	B	289	GLN
1	B	290	GLN
1	B	394	ASN
1	C	17	GLN
1	C	203	HIS
1	C	267	HIS
1	C	289	GLN
1	C	290	GLN
1	C	394	ASN

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Mol	Chain	Res	Type
1	D	203	HIS
1	D	267	HIS
1	D	289	GLN
1	D	290	GLN
1	D	394	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLG	C	3001	-	17,20,20	1.87	5 (29%)	23,28,28	2.68	10 (43%)
3	FFO	D	4002	-	28,36,36	2.48	13 (46%)	28,50,50	3.87	15 (53%)
3	FFO	B	2002	-	28,36,36	2.48	13 (46%)	28,50,50	3.90	15 (53%)
3	FFO	A	1002	-	28,36,36	2.39	13 (46%)	28,50,50	3.89	15 (53%)
2	PLG	D	4001	-	17,20,20	1.85	5 (29%)	23,28,28	2.74	11 (47%)
2	PLG	B	2001	-	17,20,20	1.91	6 (35%)	23,28,28	2.70	11 (47%)
2	PLG	A	1001	-	17,20,20	2.00	5 (29%)	23,28,28	2.68	11 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FFO	C	3002	-	28,36,36	2.40	12 (42%)	28,50,50	3.88	15 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	C	3001	-	-	3/10/12/12	0/1/1/1
3	FFO	D	4002	-	-	3/18/37/37	0/2/3/3
3	FFO	B	2002	-	-	3/18/37/37	0/2/3/3
3	FFO	A	1002	-	-	3/18/37/37	0/2/3/3
2	PLG	D	4001	-	-	2/10/12/12	0/1/1/1
2	PLG	B	2001	-	-	3/10/12/12	0/1/1/1
2	PLG	A	1001	-	-	3/10/12/12	0/1/1/1
3	FFO	C	3002	-	-	3/18/37/37	0/2/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	FFO	C4-C4A	5.49	1.49	1.41
3	D	4002	FFO	C4-C4A	5.37	1.48	1.41
3	A	1002	FFO	C4-C4A	5.18	1.48	1.41
3	C	3002	FFO	C4-C4A	5.16	1.48	1.41
2	A	1001	PLG	C4A-C4	-4.89	1.45	1.51
2	B	2001	PLG	C4A-C4	-4.66	1.45	1.51
3	D	4002	FFO	C7-N8	-4.63	1.36	1.44
3	C	3002	FFO	C7-N8	-4.59	1.37	1.44
3	D	4002	FFO	C4A-N5	4.55	1.47	1.41
2	C	3001	PLG	C4A-C4	-4.49	1.46	1.51
3	A	1002	FFO	C7-N8	-4.48	1.37	1.44
2	D	4001	PLG	C4A-C4	-4.45	1.46	1.51
3	B	2002	FFO	C7-N8	-4.44	1.37	1.44
3	B	2002	FFO	C4A-N5	4.41	1.47	1.41
3	C	3002	FFO	C4A-N5	4.31	1.47	1.41
3	A	1002	FFO	C4A-N5	4.29	1.47	1.41
3	D	4002	FFO	C13-C14	3.70	1.45	1.39
3	B	2002	FFO	C13-C14	3.61	1.45	1.39
3	A	1002	FFO	C13-C14	3.58	1.45	1.39
3	B	2002	FFO	C4-N3	3.55	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3002	FFO	C13-C14	3.47	1.45	1.39
3	A	1002	FFO	C4-N3	3.41	1.39	1.33
2	A	1001	PLG	C3-C2	3.38	1.44	1.40
3	B	2002	FFO	C2-N3	3.38	1.41	1.35
3	D	4002	FFO	C4-N3	3.35	1.38	1.33
3	D	4002	FFO	C2-N3	3.29	1.41	1.35
3	C	3002	FFO	C2-N3	3.26	1.41	1.35
3	C	3002	FFO	C4-N3	3.19	1.38	1.33
3	B	2002	FFO	CB-CA	3.13	1.57	1.53
3	D	4002	FFO	CB-CA	3.11	1.57	1.53
2	A	1001	PLG	C3-C4	3.09	1.44	1.40
2	B	2001	PLG	C3-C2	3.06	1.44	1.40
3	A	1002	FFO	C2-N3	3.02	1.40	1.35
3	D	4002	FFO	C12-C11	3.00	1.44	1.39
3	B	2002	FFO	C12-C11	2.97	1.44	1.39
2	D	4001	PLG	C3-C2	2.96	1.43	1.40
3	C	3002	FFO	C9-N10	2.94	1.51	1.45
2	D	4001	PLG	C3-C4	2.94	1.44	1.40
3	A	1002	FFO	C9-N10	2.93	1.51	1.45
2	C	3001	PLG	C3-C2	2.93	1.43	1.40
3	D	4002	FFO	C9-N10	2.91	1.51	1.45
2	C	3001	PLG	C3-C4	2.90	1.44	1.40
3	C	3002	FFO	C12-C11	2.87	1.44	1.39
3	B	2002	FFO	CB-CG	2.85	1.65	1.52
3	B	2002	FFO	C9-N10	2.81	1.51	1.45
3	A	1002	FFO	CB-CG	2.80	1.65	1.52
3	D	4002	FFO	C8A-N1	2.78	1.39	1.34
3	A	1002	FFO	C12-C11	2.77	1.44	1.39
3	A	1002	FFO	CB-CA	2.76	1.56	1.53
3	D	4002	FFO	CB-CG	2.75	1.65	1.52
3	B	2002	FFO	C8A-N1	2.73	1.39	1.34
3	C	3002	FFO	CB-CG	2.73	1.65	1.52
3	C	3002	FFO	CB-CA	2.67	1.56	1.53
3	C	3002	FFO	C8A-N1	2.64	1.39	1.34
3	A	1002	FFO	C8A-N1	2.64	1.39	1.34
3	C	3002	FFO	C7-C6	-2.64	1.49	1.52
2	B	2001	PLG	C3-C4	2.63	1.44	1.40
3	B	2002	FFO	C7-C6	-2.50	1.49	1.52
2	B	2001	PLG	O3-C3	-2.44	1.31	1.37
3	D	4002	FFO	C7-C6	-2.42	1.49	1.52
3	B	2002	FFO	CA-N	2.30	1.49	1.46
2	A	1001	PLG	C4A-N	-2.18	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4001	PLG	C6-C5	2.17	1.42	1.37
2	A	1001	PLG	C6-C5	2.16	1.42	1.37
2	B	2001	PLG	C6-C5	2.16	1.42	1.37
2	D	4001	PLG	O3-C3	-2.14	1.32	1.37
3	A	1002	FFO	C7-C6	-2.12	1.49	1.52
2	C	3001	PLG	C6-C5	2.09	1.42	1.37
2	B	2001	PLG	C4A-N	-2.08	1.36	1.46
3	D	4002	FFO	CA-N	2.07	1.49	1.46
3	A	1002	FFO	CA-N	2.04	1.49	1.46
2	C	3001	PLG	C4A-N	-2.04	1.36	1.46

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1002	FFO	NA2-C2-N1	9.22	131.59	117.25
3	B	2002	FFO	NA2-C2-N1	9.15	131.48	117.25
3	C	3002	FFO	NA2-C2-N1	9.11	131.43	117.25
3	D	4002	FFO	NA2-C2-N1	9.11	131.41	117.25
3	A	1002	FFO	C4-N3-C2	7.18	127.34	115.93
3	C	3002	FFO	C4-N3-C2	7.10	127.22	115.93
3	B	2002	FFO	C4-N3-C2	7.09	127.20	115.93
3	D	4002	FFO	C4-N3-C2	7.07	127.16	115.93
3	B	2002	FFO	N3-C2-N1	-7.00	114.44	125.42
3	C	3002	FFO	N3-C2-N1	-6.98	114.48	125.42
3	A	1002	FFO	N3-C2-N1	-6.96	114.50	125.42
3	D	4002	FFO	N3-C2-N1	-6.86	114.66	125.42
3	B	2002	FFO	C15-C14-C13	6.12	127.41	119.03
3	C	3002	FFO	C15-C14-C13	6.12	127.41	119.03
3	D	4002	FFO	C15-C14-C13	6.08	127.36	119.03
3	A	1002	FFO	C15-C14-C13	6.06	127.32	119.03
3	C	3002	FFO	C16-C15-C14	-5.52	113.92	120.30
3	D	4002	FFO	C16-C15-C14	-5.52	113.92	120.30
3	B	2002	FFO	C16-C15-C14	-5.50	113.94	120.30
2	D	4001	PLG	C4-C4A-N	5.49	121.84	111.58
3	A	1002	FFO	C16-C15-C14	-5.48	113.97	120.30
2	B	2001	PLG	C4-C4A-N	5.34	121.55	111.58
2	C	3001	PLG	C4-C4A-N	5.28	121.45	111.58
3	A	1002	FFO	O5B-C5A-N5	-5.14	117.92	125.36
3	B	2002	FFO	CB-CG-CD	5.10	124.55	113.59
2	A	1001	PLG	C4-C4A-N	5.09	121.09	111.58
3	B	2002	FFO	O5B-C5A-N5	-5.08	118.01	125.36
3	D	4002	FFO	CB-CG-CD	5.08	124.50	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3002	FFO	O5B-C5A-N5	-5.02	118.09	125.36
2	A	1001	PLG	C2A-C2-C3	4.96	127.01	120.89
3	D	4002	FFO	O5B-C5A-N5	-4.93	118.22	125.36
3	C	3002	FFO	CB-CG-CD	4.91	124.13	113.59
3	A	1002	FFO	CB-CG-CD	4.90	124.12	113.59
2	D	4001	PLG	C2A-C2-C3	4.82	126.84	120.89
2	B	2001	PLG	C2A-C2-C3	4.80	126.82	120.89
2	D	4001	PLG	CA-N-C4A	4.79	124.62	112.54
2	D	4001	PLG	OP4-C5A-C5	4.74	118.39	109.35
2	C	3001	PLG	C2A-C2-C3	4.70	126.70	120.89
2	B	2001	PLG	OP4-C5A-C5	4.61	118.14	109.35
2	C	3001	PLG	OP4-C5A-C5	4.58	118.08	109.35
2	A	1001	PLG	OP4-C5A-C5	4.58	118.07	109.35
2	B	2001	PLG	CA-N-C4A	4.52	123.93	112.54
2	C	3001	PLG	CA-N-C4A	4.49	123.87	112.54
2	A	1001	PLG	CA-N-C4A	4.40	123.62	112.54
3	B	2002	FFO	C4A-N5-C6	-4.39	111.53	119.31
3	C	3002	FFO	C4A-N5-C6	-4.37	111.55	119.31
3	D	4002	FFO	C4A-N5-C6	-4.36	111.58	119.31
3	A	1002	FFO	C4A-N5-C6	-4.29	111.70	119.31
3	C	3002	FFO	C13-C14-N10	-4.27	112.11	120.97
3	B	2002	FFO	C13-C14-N10	-4.24	112.18	120.97
3	A	1002	FFO	C13-C14-N10	-4.24	112.19	120.97
3	A	1002	FFO	C2-N1-C8A	4.23	124.01	114.54
3	D	4002	FFO	C13-C14-N10	-4.22	112.23	120.97
3	C	3002	FFO	C2-N1-C8A	4.19	123.94	114.54
3	B	2002	FFO	C2-N1-C8A	4.18	123.90	114.54
3	D	4002	FFO	C2-N1-C8A	4.14	123.82	114.54
3	B	2002	FFO	C12-C13-C14	-3.77	115.94	120.30
3	A	1002	FFO	C4A-C4-N3	-3.76	115.41	123.14
3	B	2002	FFO	C4A-C4-N3	-3.76	115.42	123.14
2	D	4001	PLG	C6-N1-C2	3.75	126.11	119.17
3	C	3002	FFO	C12-C13-C14	-3.75	115.97	120.30
3	D	4002	FFO	C4A-C4-N3	-3.74	115.46	123.14
2	A	1001	PLG	C6-N1-C2	3.72	126.06	119.17
2	B	2001	PLG	C6-N1-C2	3.72	126.06	119.17
3	C	3002	FFO	C4A-C4-N3	-3.71	115.51	123.14
2	C	3001	PLG	C5A-C5-C6	-3.71	113.27	119.37
3	D	4002	FFO	C12-C13-C14	-3.67	116.05	120.30
3	A	1002	FFO	C12-C13-C14	-3.67	116.06	120.30
2	A	1001	PLG	C5A-C5-C6	-3.67	113.34	119.37
2	D	4001	PLG	C5A-C5-C6	-3.66	113.35	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3001	PLG	C6-N1-C2	3.66	125.94	119.17
2	B	2001	PLG	C5A-C5-C6	-3.55	113.53	119.37
2	B	2001	PLG	C3-C2-N1	-3.41	116.37	120.77
2	D	4001	PLG	C3-C2-N1	-3.38	116.41	120.77
3	B	2002	FFO	C4-C4A-C8A	3.29	117.01	114.44
3	D	4002	FFO	C4-C4A-C8A	3.29	117.01	114.44
2	C	3001	PLG	C3-C2-N1	-3.25	116.57	120.77
2	A	1001	PLG	C3-C2-N1	-3.25	116.58	120.77
2	A	1001	PLG	C3-C4-C5	3.24	121.83	118.72
2	C	3001	PLG	C3-C4-C5	3.22	121.81	118.72
3	C	3002	FFO	C4-C4A-C8A	3.22	116.96	114.44
2	B	2001	PLG	C3-C4-C5	3.21	121.80	118.72
2	D	4001	PLG	C3-C4-C5	3.17	121.76	118.72
3	A	1002	FFO	C4-C4A-C8A	3.15	116.90	114.44
2	B	2001	PLG	OP3-P-OP4	2.50	113.37	106.73
3	B	2002	FFO	C11-C-N	2.46	121.77	117.06
2	C	3001	PLG	OP3-P-OP4	2.43	113.19	106.73
2	A	1001	PLG	OP3-P-OP4	2.41	113.15	106.73
2	B	2001	PLG	C5-C6-N1	-2.36	119.89	123.82
2	C	3001	PLG	C5-C6-N1	-2.36	119.89	123.82
2	A	1001	PLG	C5-C6-N1	-2.35	119.90	123.82
3	D	4002	FFO	C11-C-N	2.35	121.56	117.06
3	A	1002	FFO	C11-C-N	2.34	121.54	117.06
2	D	4001	PLG	C5-C6-N1	-2.33	119.93	123.82
3	C	3002	FFO	C11-C-N	2.32	121.52	117.06
2	D	4001	PLG	OP3-P-OP4	2.24	112.70	106.73
3	A	1002	FFO	NA2-C2-N3	-2.15	113.91	117.25
3	D	4002	FFO	NA2-C2-N3	-2.14	113.92	117.25
2	D	4001	PLG	C6-C5-C4	-2.08	116.65	118.12
3	B	2002	FFO	NA2-C2-N3	-2.04	114.07	117.25
3	C	3002	FFO	NA2-C2-N3	-2.03	114.10	117.25
2	A	1001	PLG	C4A-C4-C3	-2.01	117.89	120.04
2	B	2001	PLG	C4A-C4-C3	-2.00	117.90	120.04

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3001	PLG	C5-C4-C4A-N
2	D	4001	PLG	C5-C4-C4A-N
2	B	2001	PLG	C5-C4-C4A-N
2	A	1001	PLG	C5-C4-C4A-N

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Mol	Chain	Res	Type	Atoms
2	C	3001	PLG	C3-C4-C4A-N
2	D	4001	PLG	C3-C4-C4A-N
2	B	2001	PLG	C3-C4-C4A-N
2	A	1001	PLG	C3-C4-C4A-N
3	A	1002	FFO	N-CA-CB-CG
3	B	2002	FFO	N-CA-CB-CG
3	C	3002	FFO	N-CA-CB-CG
3	D	4002	FFO	N-CA-CB-CG
3	B	2002	FFO	C13-C14-N10-C9
3	A	1002	FFO	C13-C14-N10-C9
3	D	4002	FFO	C13-C14-N10-C9
3	A	1002	FFO	C15-C14-N10-C9
3	C	3002	FFO	C13-C14-N10-C9
3	B	2002	FFO	C15-C14-N10-C9
2	C	3001	PLG	C5A-OP4-P-OP3
2	B	2001	PLG	C5A-OP4-P-OP3
2	A	1001	PLG	C5A-OP4-P-OP3
3	D	4002	FFO	C15-C14-N10-C9
3	C	3002	FFO	C15-C14-N10-C9

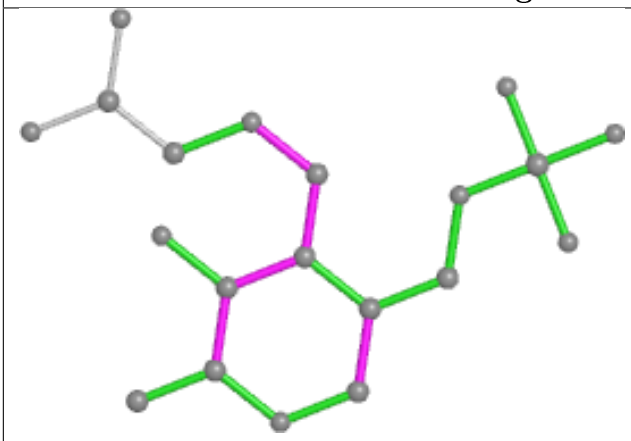
There are no ring outliers.

2 monomers are involved in 2 short contacts:

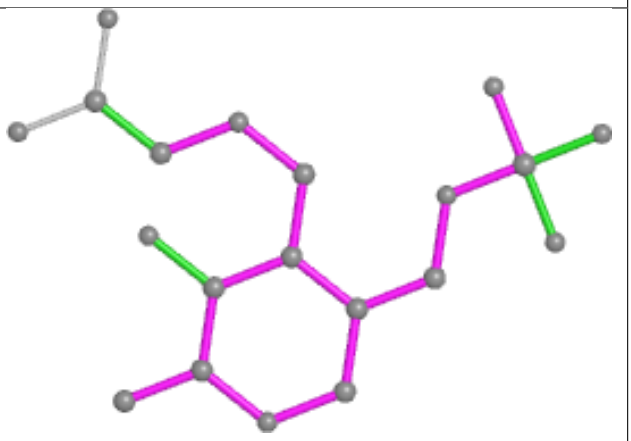
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	PLG	1	0
2	A	1001	PLG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

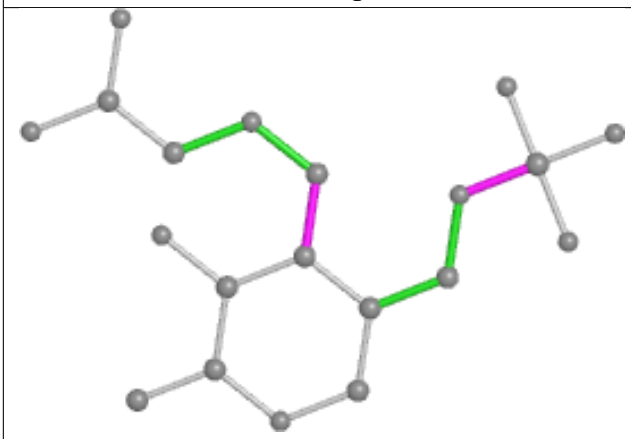
Ligand PLG C 3001



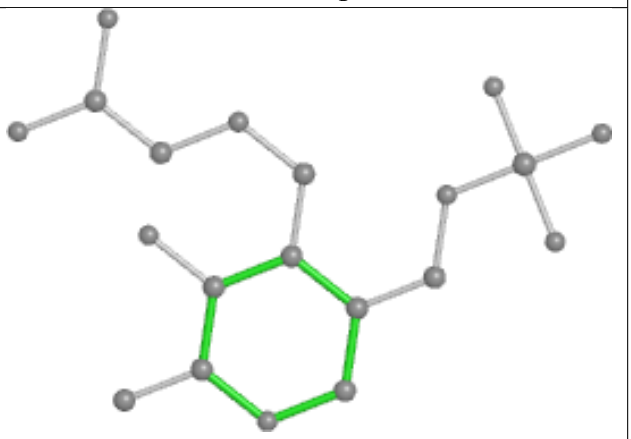
Bond lengths



Bond angles

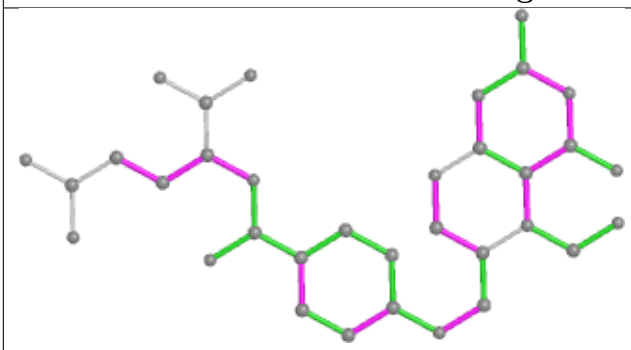


Torsions



Rings

Ligand FFO D 4002



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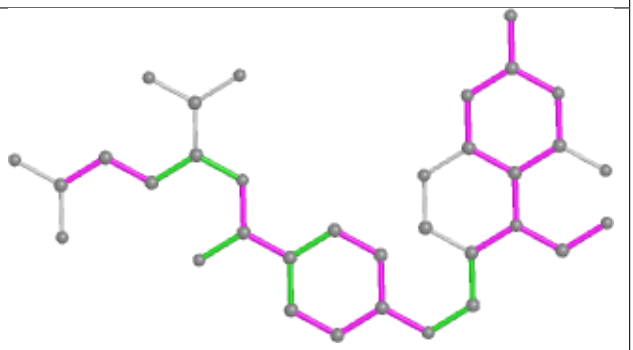

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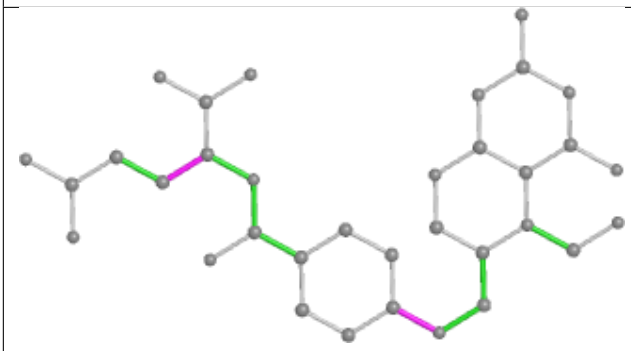
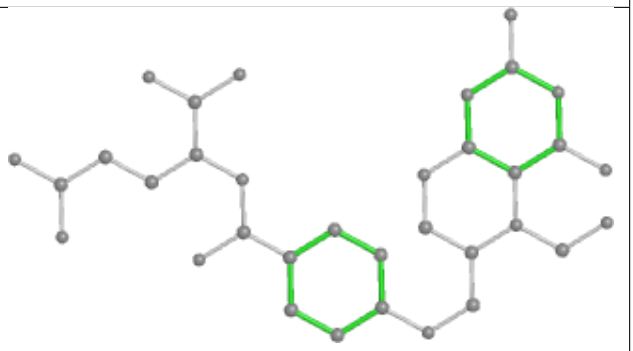
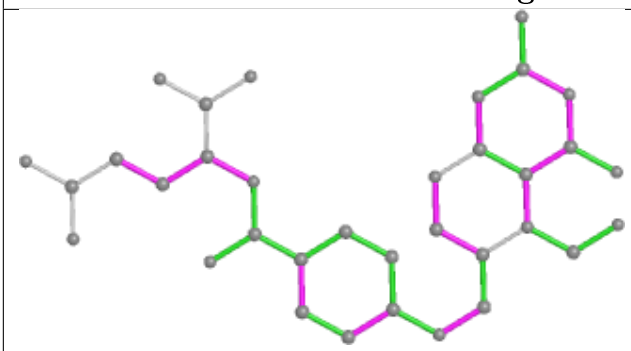


Torsions

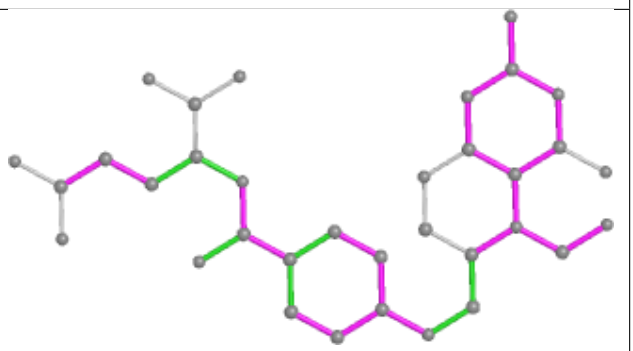


Rings

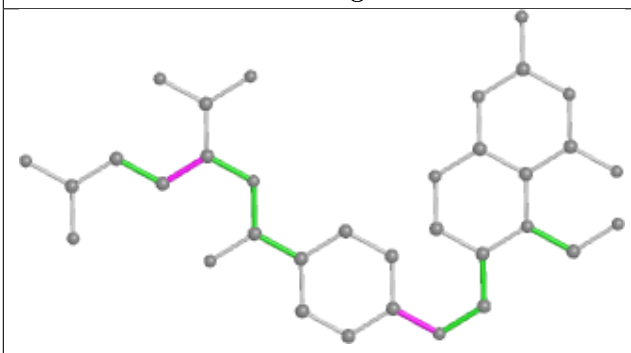
Ligand FFO B 2002



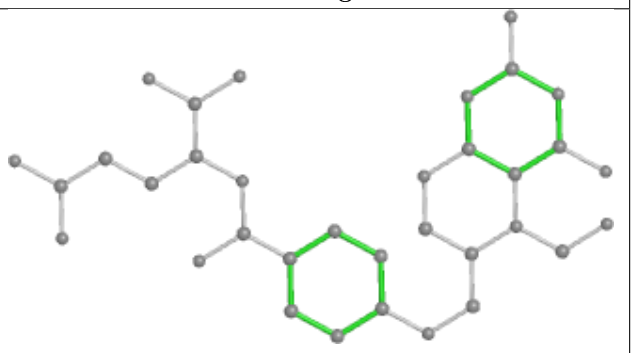
Bond lengths



Bond angles

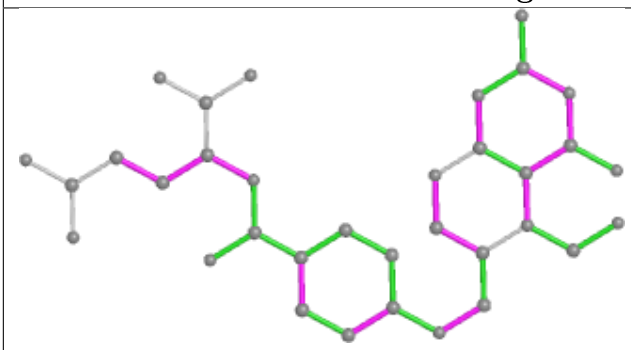


Torsions

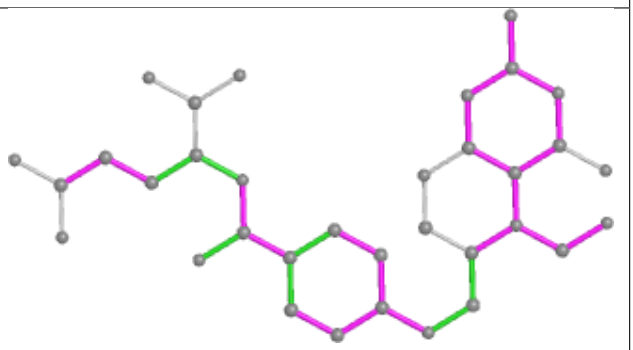


Rings

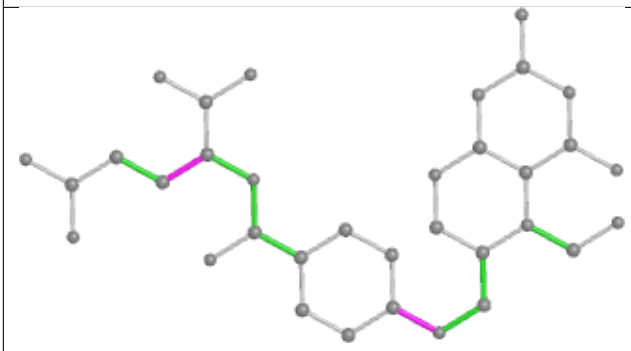
Ligand FFO A 1002



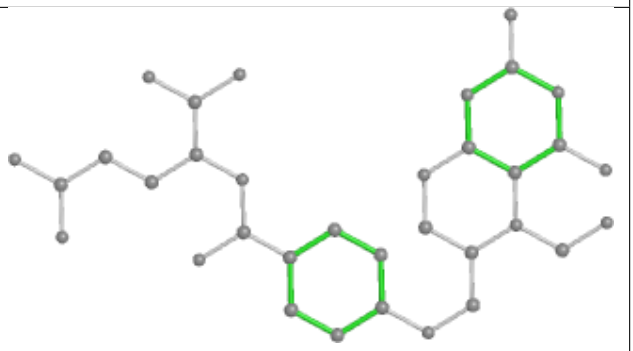
Bond lengths



Bond angles

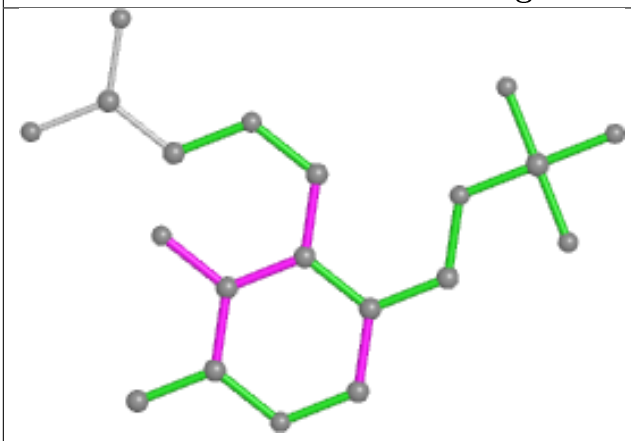


Torsions

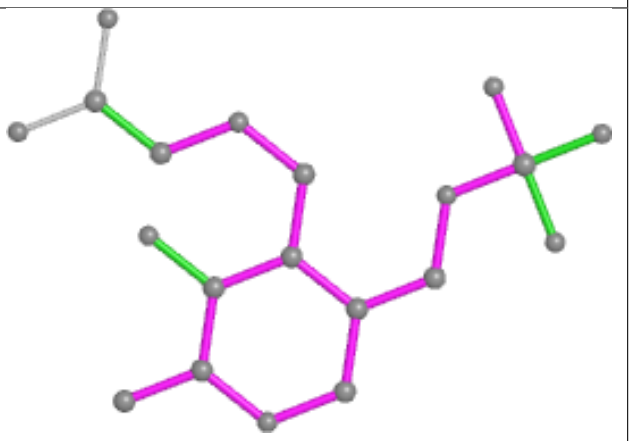


Rings

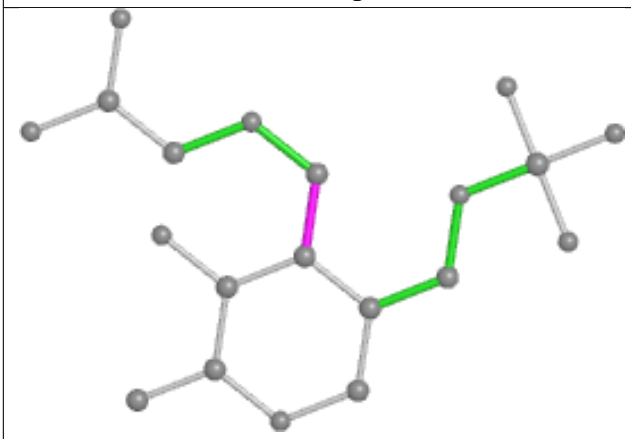
Ligand PLG D 4001



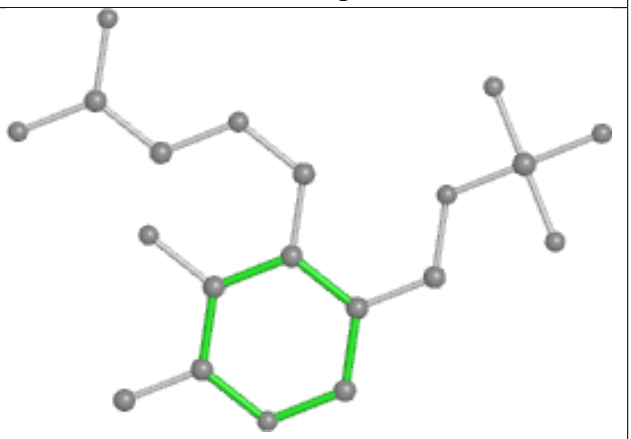
Bond lengths



Bond angles

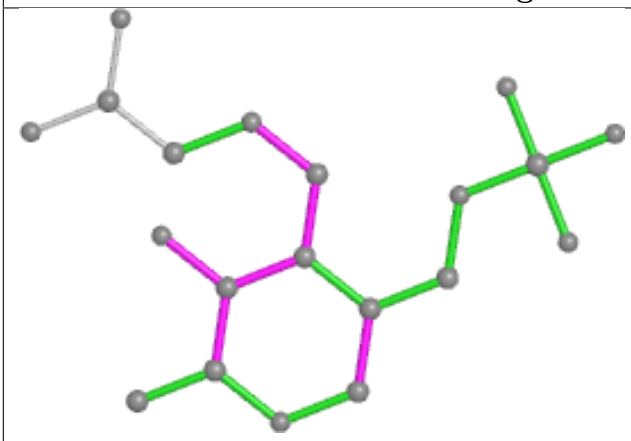


Torsions

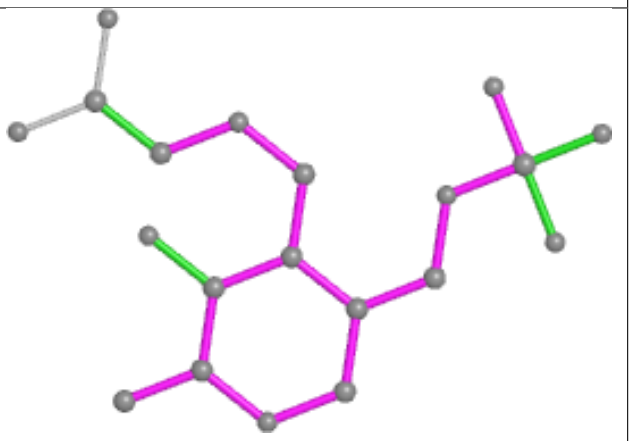


Rings

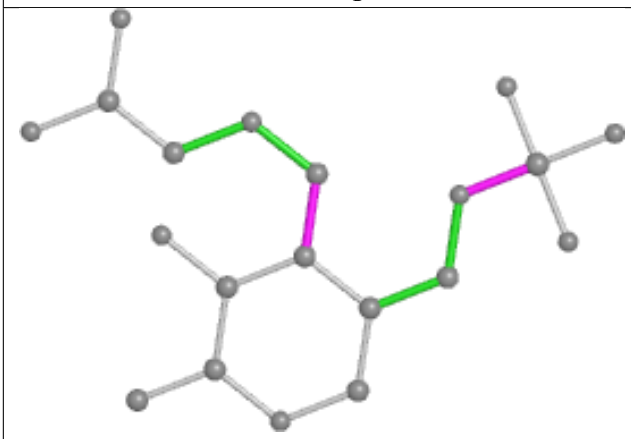
Ligand PLG B 2001



Bond lengths



Bond angles



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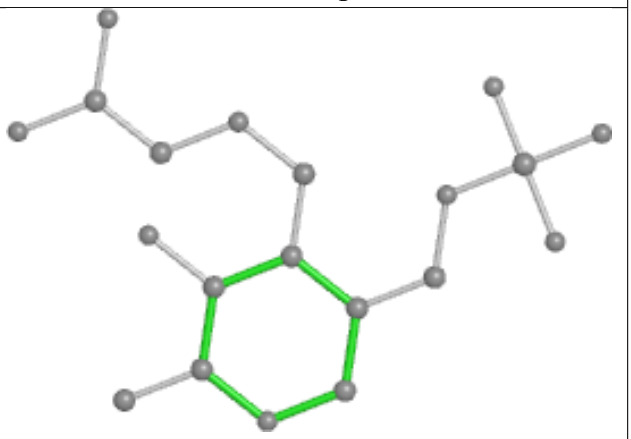
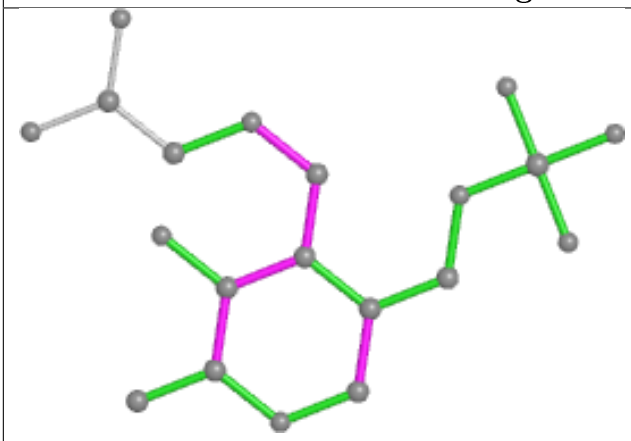
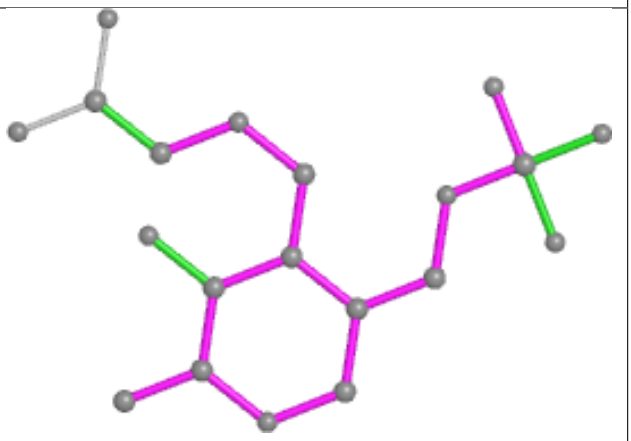


Rings

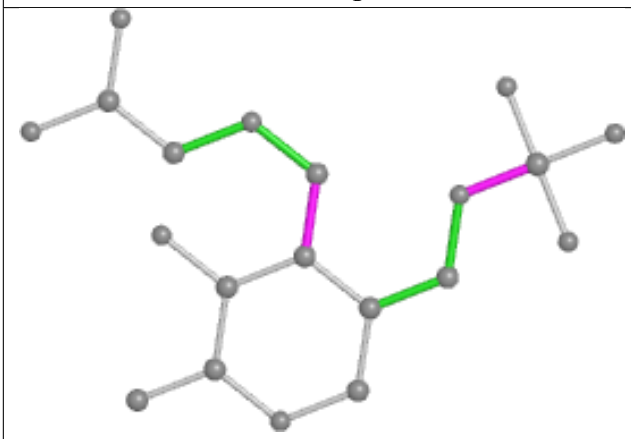
Ligand PLG A 1001



Bond lengths



Bond angles



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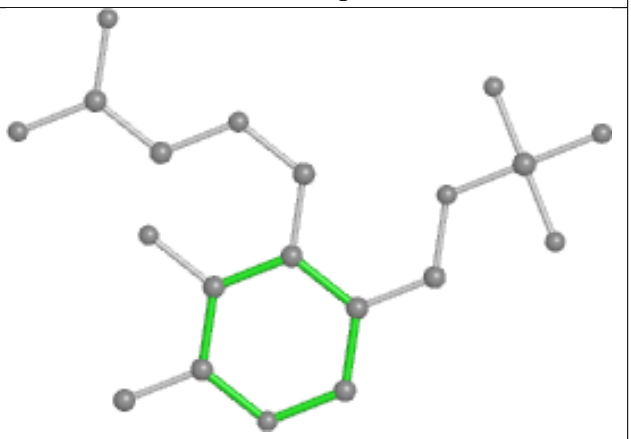
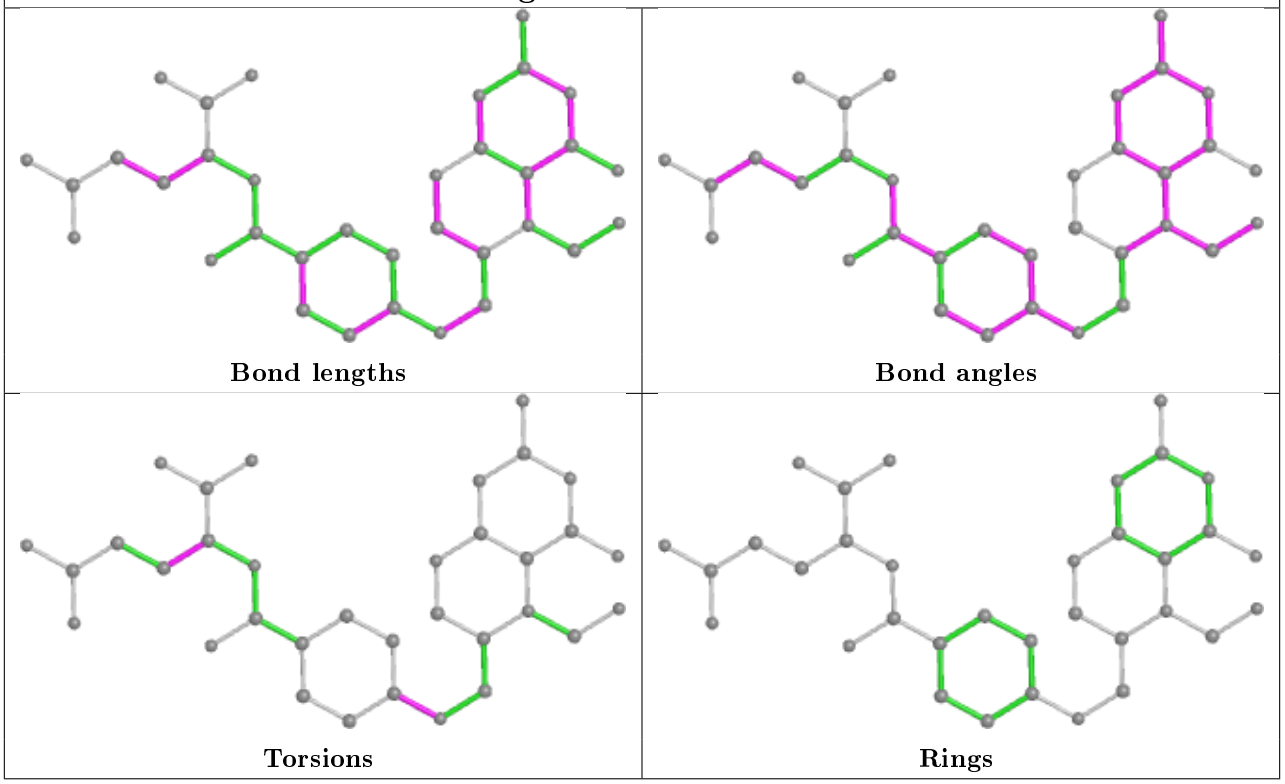


Rings

Ligand FFO C 3002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	416/417 (99%)	-0.04	0	100	100	22, 33, 52, 69	0
1	B	417/417 (100%)	-0.03	0	100	100	21, 33, 54, 66	0
1	C	417/417 (100%)	-0.07	0	100	100	21, 36, 55, 70	0
1	D	416/417 (99%)	-0.02	0	100	100	22, 33, 53, 67	0
All	All	1666/1668 (99%)	-0.04	0	100	100	21, 34, 54, 70	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FFO	B	2002	34/34	0.93	0.18	37,41,58,63	0
3	FFO	D	4002	34/34	0.94	0.19	35,41,60,64	0
3	FFO	C	3002	34/34	0.94	0.19	29,41,52,57	0
3	FFO	A	1002	34/34	0.95	0.18	28,39,49,54	0

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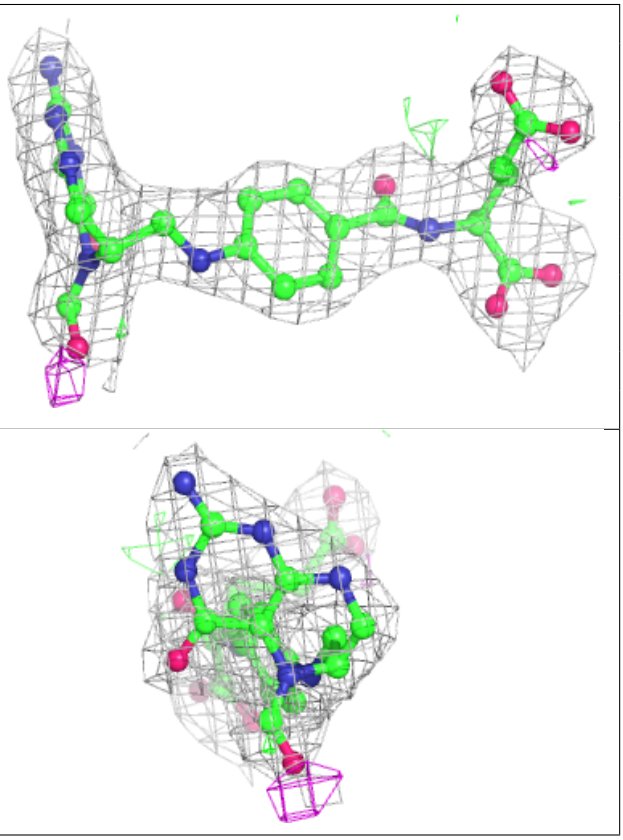
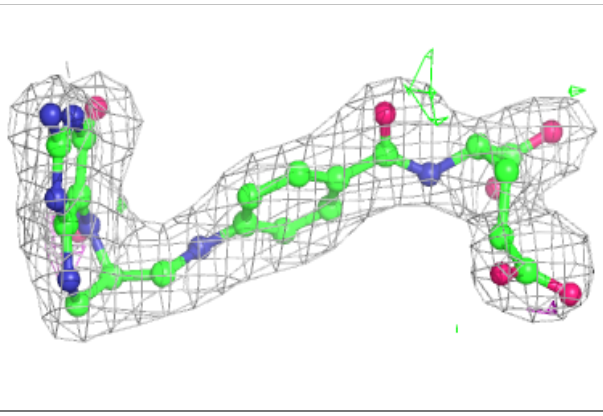
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLG	B	2001	20/20	0.98	0.19	27,30,36,36	0
2	PLG	A	1001	20/20	0.98	0.17	25,28,31,32	0
2	PLG	D	4001	20/20	0.98	0.18	26,30,34,37	0
2	PLG	C	3001	20/20	0.99	0.17	25,29,34,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FFO B 2002:

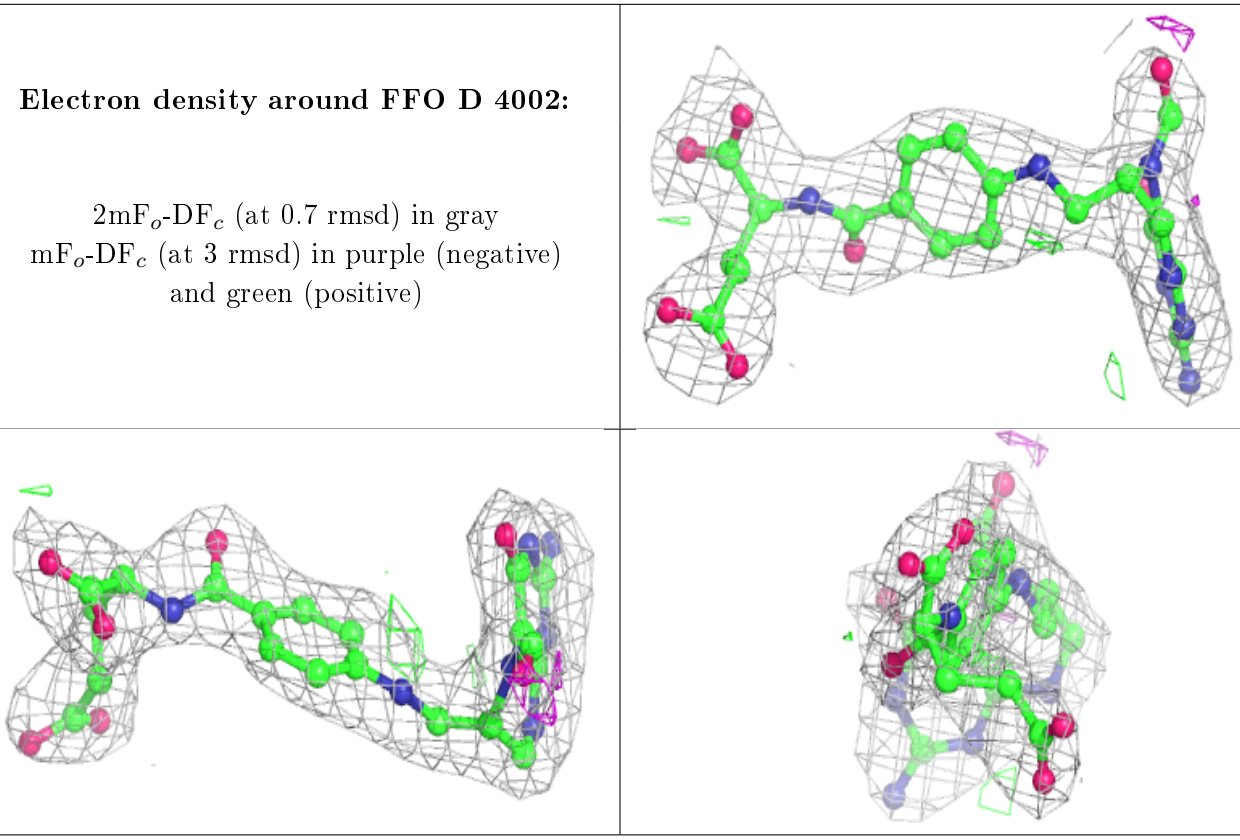
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





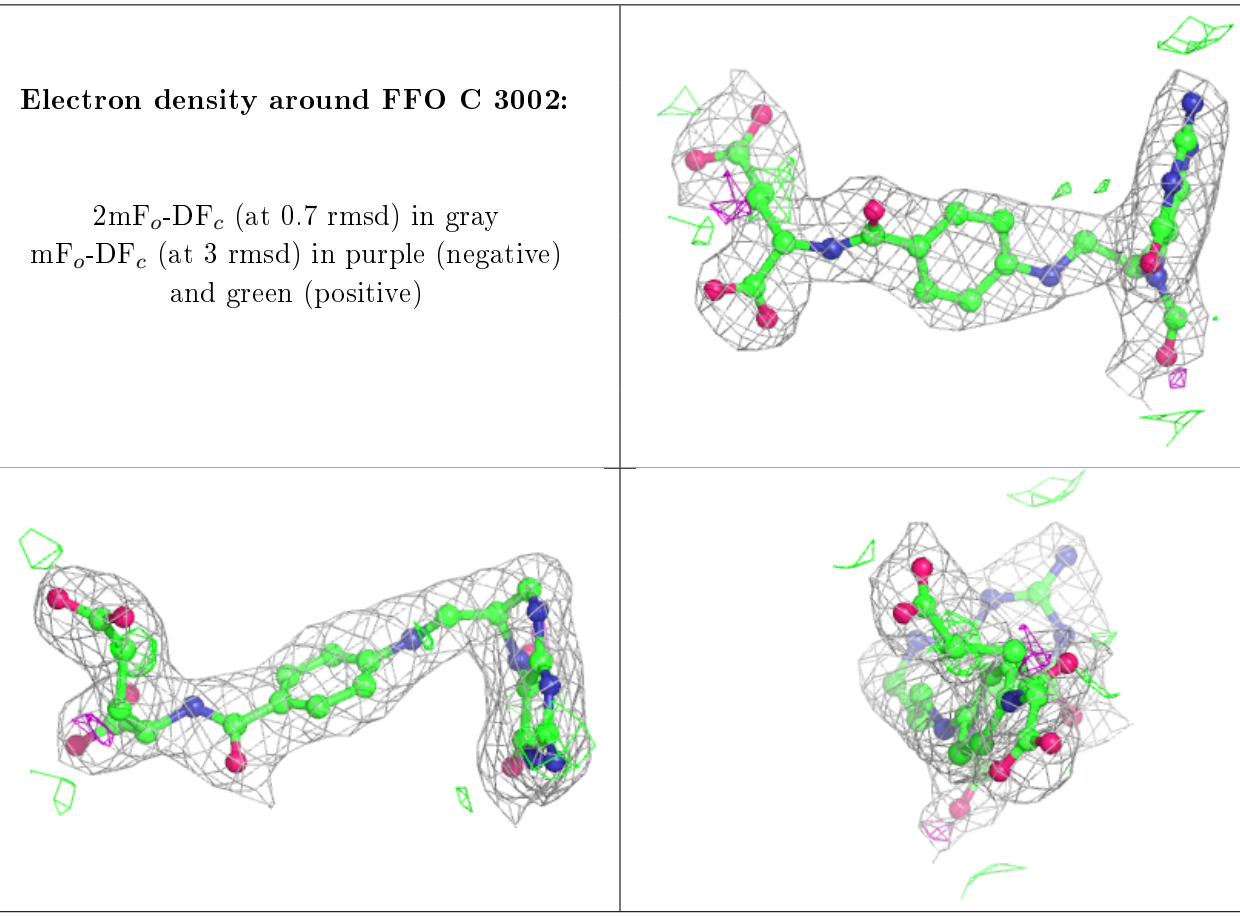
Electron density around FFO D 4002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



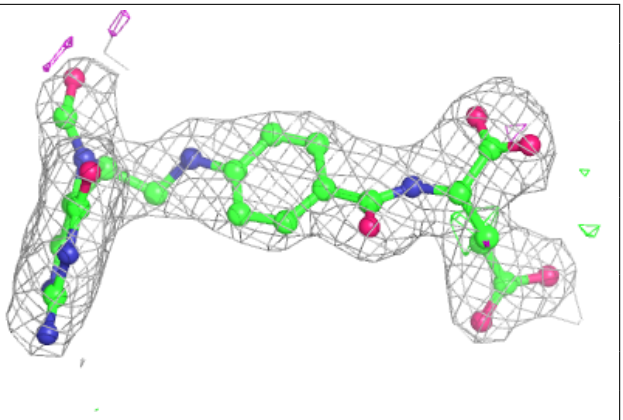
Electron density around FFO C 3002:

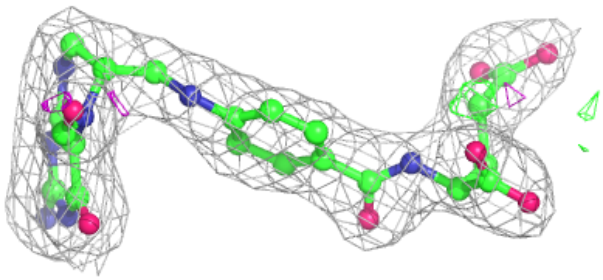
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

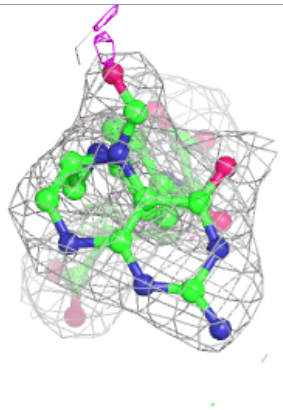


Electron density around FFO A 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

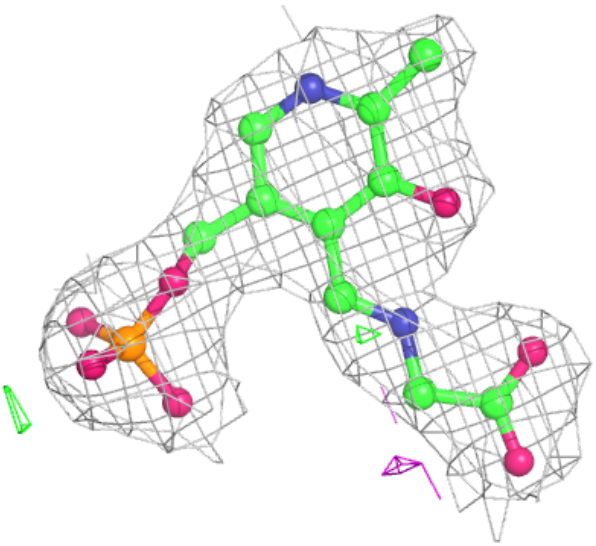


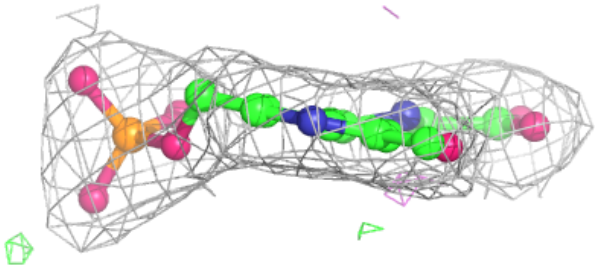


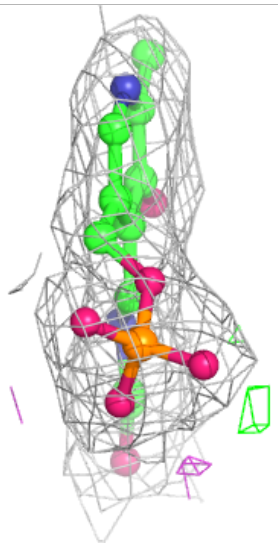


Electron density around PLG B 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

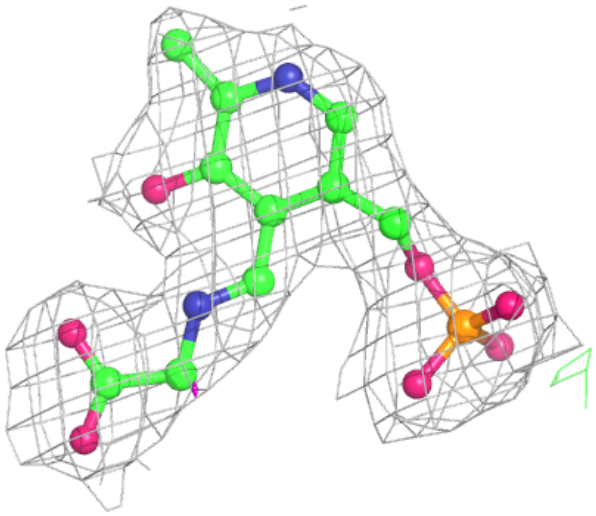


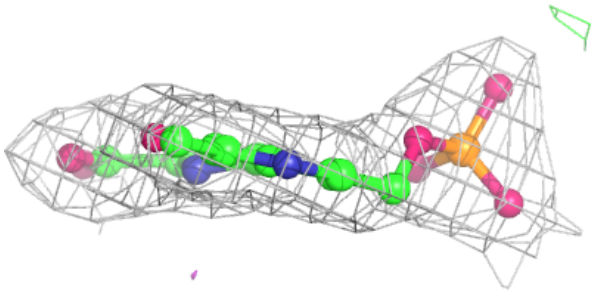


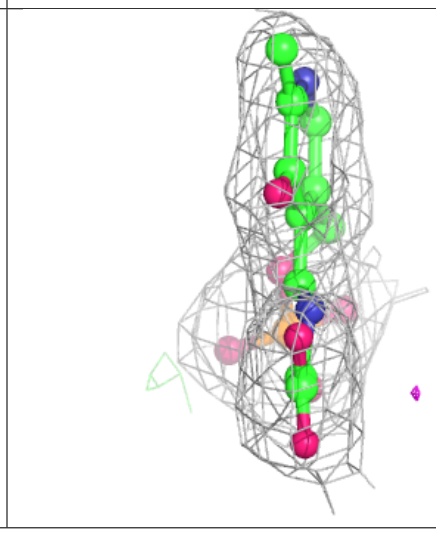


Electron density around PLG A 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

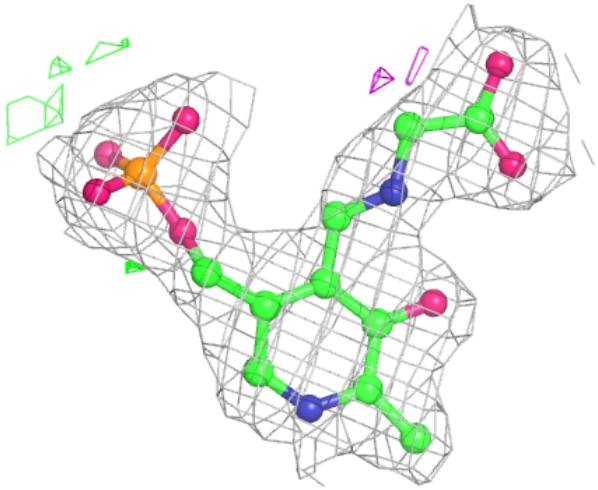


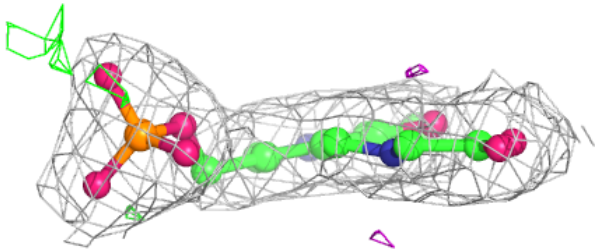


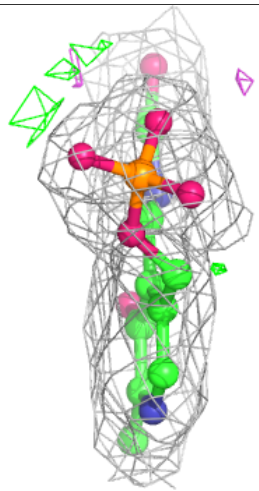


Electron density around PLG D 4001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

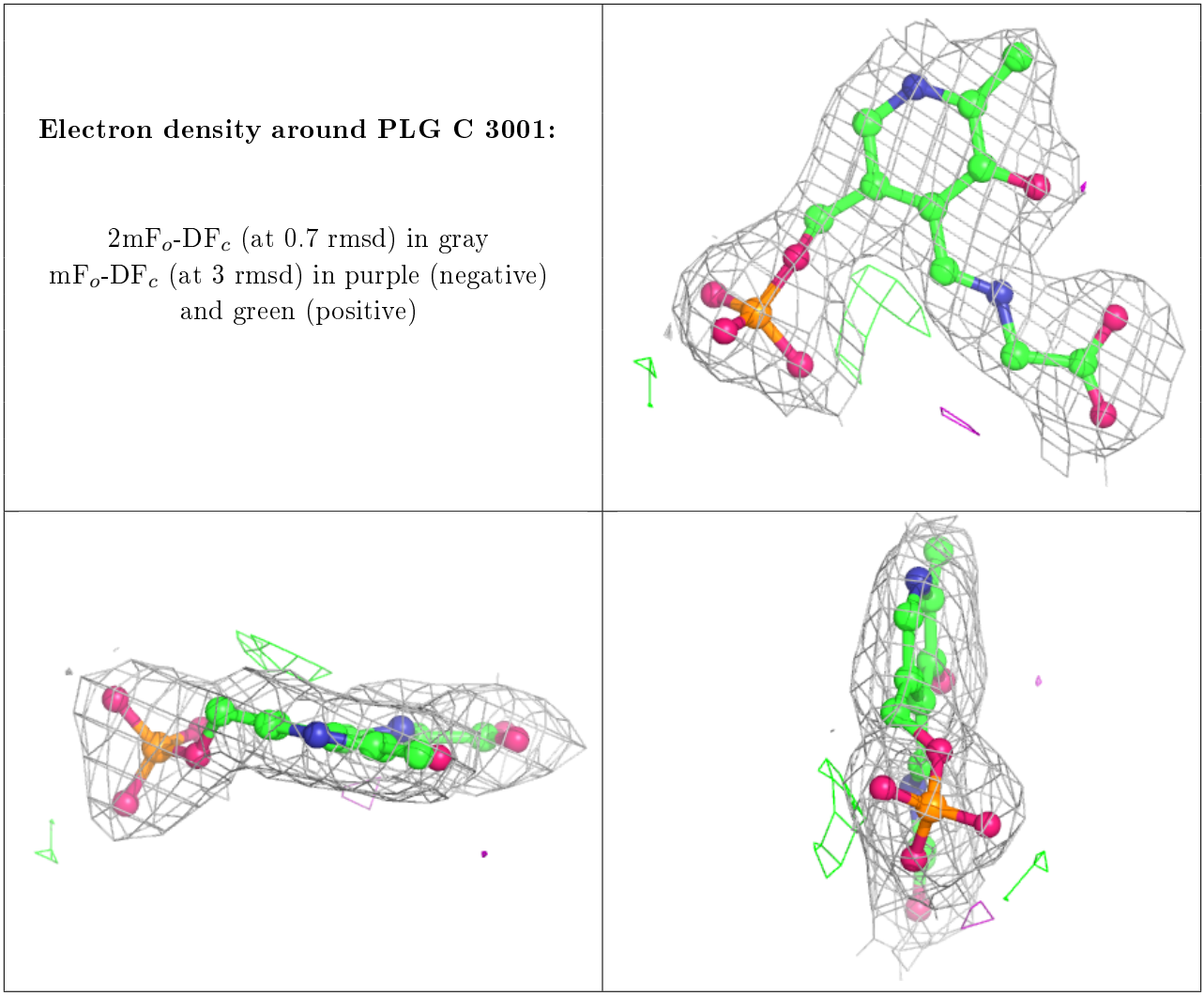






Electron density around PLG C 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.